APPENDIX C
DETERMINING APPROPRIATE SCALE AND SPATIAL RESOLUTION

This appendix is an example of a detailed approach for defining the level of spatial complexity (*i.e.*, location, size, and number of parcels) in a TRIM.FaTE analysis. There are many factors that influence scenario complexity, including the characteristics of the pollutant, the environmental setting, the exposed population, the impact of interest, the available data, and available computer resources. A clear analysis objective offers a starting point for setting up the scenario with an appropriate level of complexity. The TRIM.FaTE modeling framework uses a system where the analysis objective is classified into one of three basic types. For each type of objective, a series of questions can be used to identify the natural and artificial boundaries of the system. A preliminary decision tree is developed for each objective type to assist the user in determining which boundary or set of boundaries is appropriate for a given modeling objective. The decision trees are used to provide a standard approach for setting up a simulation.

After the initial scenario is constructed and a simulation has been completed, the preliminary results need to be evaluated to confirm that the most appropriate scale has been used. The methodology for determining appropriate scale and spatial resolution as well as suggestions for defining compartments are included in this chapter.

There are several questions that need to be answered before the appropriate level of scenario complexity can be determined. As with any modeling exercise, the first and foremost step in a TRIM.FaTE analysis is to clearly state the objective of the analysis. The objective should identify the chemical(s) of concern, the exposed population (individual, species, population, cohort, or environmental compartment), and the health endpoint (chronic or acute) to be assessed. The exposed population, either human or ecological, or landscape component (*e.g.*, lake, wetland, agricultural plot), is referred as the **target**. This section presents a tiered approach that incorporates all of these objectives to define the appropriate scale and resolution of a given TRIM.FaTE scenario.

For the chemical(s) of concern, the two most important factors for determining the appropriate modeling scale are how rapidly the chemical moves and how rapidly the chemical degrades in the environment. The range of mobility for each target of interest also needs to be considered. In addition to providing information about modeling scale, the mobility characteristics of the target help determine the appropriate level of resolution of the scenario. Finally, the endpoint being assessed will provide important information about both temporal and spatial scale of the scenario.

The approach described in the following section generates a starting point for any given analysis objective for which TRIM.FaTE is designed, and is intended to impart some consistency and transparency into the scenario set up process. Additionally, once a scale has been chosen, one must determine if that scale is appropriate when compared to other sources of model uncertainty.

C.1 CLASSIFICATION OF THE ANALYSIS OBJECTIVE

The methodology for the set up of a scenario will depend largely on the mobility of the target. The mobility of each exposed population is categorized into one of three general classes: mobile, bounded, and stationary. Each class is described in the following sections and summarized in Table C-1. Depending on which category best describes the target of interest, the user is referred to one of three binary decision trees that are described in Section C.2. The decision trees provide a series of questions that help the user determine the appropriate set of boundaries and parcels in the analysis. Information on the different boundary types is provided in Section C.2.

Table C-1
Classification of Modeling Objectives Based on Target of Interest

Target Class	Description	Rationale and Example
Mobile	Highly mobile cohorts, individuals, animals or organisms	Concentration in air resulting from point source will decline with distance traveled from source. If a child goes to school near a source but lives farther from the source and plays in a park somewhere else then one would want to maximize resolution within the model system.
Bounded	Animals with a limited range or habitat	Red tailed hawks or land mammals in a limited or bounded habitat that is a fixed distance from the source. Concentrations or environmental conditions may vary across the habitat/range but highly resolved concentration gradients between the source and the study area are not necessary.
Stationary	Fixed location in space that may be influenced by its surroundings but does not move relative to source	Forest, pond, agricultural plot, wetlands. Consider chemical transfer from adjacent areas (watershed, air parcel).

C.1.1 MOBILE EXPOSED POPULATIONS

The first target class is referred to as **mobile**. This class includes humans and large animals that are highly mobile and can freely move about the region impacted by the source(s). Mobile targets require maximum resolution when estimating concentration, especially for areas where the highest exposure is likely to occur or with a high likelihood of occupancy by the target (schools, residential areas, wintering grounds). Each scenario focused on mobile targets should be designed to provide maximum possible resolution, given the constraints of limited computing resources, model uncertainty, and measurement imprecision.

C.1.2 BOUNDED EXPOSED POPULATIONS

The second target class is referred to as **bounded**. This class includes targets that are expected to have some limits, either natural or artificial, on their habitat or mobility range. For example, red tailed hawks that hunt and live in a specific orchard or fish confined to a certain lake or pond would be included in this class. The scale and resolution of a given scenario should be selected to provide the desired level of detail within the bounded region. Areas outside the bounded region can be simplified to include only the information that influences transport of chemical into the region of interest. For example, if one region has a high quantity of vegetation and the chemical has a high degradation rate in vegetation, this would be considered separately because it influences the mass balance. The bounded area where the target(s) reside may or may not be well mixed (*i.e.*, the concentration across the area does not change significantly). If the range is not expected to be well mixed, more spatial resolution within the range can be included, provided it can be justified under the constraints of model uncertainty. If the range is well mixed then additional spatial resolution is not necessary.

C.1.3 STATIONARY EXPOSED POPULATIONS

The third target class is referred to as **stationary**. This class includes all immobile targets such as lakes, forests, agricultural plots, or wetlands. Stationary targets also require little resolution between the source and the target. Only information that relates the point source to the location of interest is necessary. Such information might include adjacent air parcels and drainage areas from which water (runoff) and soil (erosion) are transferred to the stationary target.

When more than one target is considered in the analysis, the scenario should be set up to satisfy the target that requires the most resolution. For example, if a study was interested in both the exposure received by a cohort of humans (mobile target) and the maximum concentration in a local pond (stationary target), the setup should follow the procedure described in the decision tree for the mobile target. The concentration in the pond will likely be estimated in the process of characterizing the various human exposure pathways. Thus, the "high resolution" system based on the mobile target should provide an adequate level of detail for estimating the concentration in the pond. If the concentration in the pond were not determined by the system for the mobile target, the user could either add additional parcels to the scenario to account for the pond or set up an additional analysis based on the stationary target.

C.2 PARCEL BOUNDARY TYPES

The decision trees for each of the target classes use existing information about boundaries of the modeling system to facilitate the set up of a scenario. There are several types of these boundaries that can be used independently or in concert. For simplicity, three classes of boundaries are defined: natural boundaries, physiochemical boundaries, and population boundaries. Each of the boundary types is summarized below along with a description of how they are used to define system boundaries and parcels. The boundary types are summarized in Table C-2. These simple classifications allow the boundary types to be easily referenced from the binary decision trees.

Table C-2
Boundary Types Coded for Use in Decision Trees

CODE	BOUNDARY TYPE
1	**Natural**
1a	Air shed
1b	Water shed
1c	Lakes and rivers
1d	Homogeneous land use/cover regions
2	**Physiochemical**
2a	Characteristic travel distance
2b	Dispersion modeling
2max	External boundary capturing 90 % of chemical mass (system boundary)
3	**Population**
3a	Semi-mobile (range)
3b	Immobile (location)

C.2.1 NATURAL BOUNDARIES

Natural boundaries include air sheds, watersheds, water bodies and homogeneous land use and land cover regions. When specifying natural boundaries one can refer to satellite images, topographical maps, or GIS coverage databases.

An air shed can include large valleys such as the Sacramento valley (CA) where, due to inversion layers and diurnal wind patterns, the air mass is confined and well mixed throughout the area for a large portion of the time. Air shed boundaries can also include smaller valleys when meteorological conditions produce long residence time for the air mass in the bounded region. Air shed boundaries are useful in providing information about the scale of the model region (*i.e.*, external boundaries of the system).

Watersheds are also useful in determining the scale of the system as well as the size and location of parcels within the system, especially if the concentration in a particular lake or wetland is of interest. Watershed boundaries can be identified or approximated from topographical maps by tracing ridgelines and noting the origin and direction of flow for streams and rivers. The size and location of a watershed can influence the transfer of chemical to water bodies within the basin.

Locations and sizes of water bodies and information describing land use and land cover patterns can also indicate important boundaries in the system. If the analysis objective includes estimating the impact of a source on a particular water body, agricultural plot, or forest, these boundaries can be incorporated into the scenario setup.

C.2.2 PHYSICOCHEMICAL BOUNDARIES

Physicochemical boundaries are based on the characteristic travel distance and direction of the chemical of interest. Physicochemical boundaries can help define both internal parcels and system scale. Physiochemical boundaries can be applied to water bodies, such as rivers and streams, if advection and diffusion in water is the dominant pathway by which a chemical travels through the environment, but the default translocation pathway for most chemicals will be advection in the air.

When determining the scale of the external system boundaries, the user needs to determine the range over which the contaminant is likely to spread and if it is necessary for the model system to capture this range for the user to be able to answer the desired question. For example, chemicals that are highly mobile in the environment will move far from the source. One might want to include this entire range, for example, if they want to determine the total number of people exposed to the chemical. If the goal is to determine the exposure to a nearby population, a smaller system might be appropriate. In this case, a background concentration will need to be used to account for pollutant mass flowing back into the system when there is a change in the wind direction. For chemicals that rapidly deposit to the land surface, it is often easier to model the range over which the chemical is likely to spread and thus is desirable to model the full range of the chemical.

Travel distance (based on the chemical-specific deposition velocity), local weather data (*e.g.*, wind speed/direction, rainfall data, temperature), and approximate landscape characteristics (*e.g.*, locations of water, forest, and bare soil) are used to provide an estimate of the distance that a chemical will travel from the source. Ideally, one needs to account for the travel distance in each of the four major directions (*i.e.*, north, south, east, and west) to account for variations resulting from land use and changing weather patterns. The travel distance can be used to estimate changes in atmospheric concentration, thus providing the maximum resolution that can still be considered statistically significant (can be detected given the uncertainty in model predictions and imprecision in environmental measurements). Characteristic travel distance can be used to construct polygons that incorporate advection, dispersion, and physical loss of chemical from the atmosphere.

If the objective is to track the movement and fate of the pollutant over its lifetime then one would want to calculate the distance over which 90 percent of the pollution had been removed from the air by reactions and dry deposition.

The size of a grid cell can then be determined by calculating the length over which X percent of the mass of the chemical species with the shortest characteristic distance is lost. One would want to base this on both atmospheric reactions and the most rapid depositional processes (*i.e.,* assume both wet and dry deposition). The selection of a factor of X = 50 is dependent on

the precision of the model output and relevant measurements and will likely result in grid cells that are smaller than necessary. The following equation can be used to approximate the distance, L, for any specified percent reduction:

$$L = -\ln((100 - \%\ \text{reduction}) / 100) * \text{characteristic length}$$

where:

% reduction = the specified percent change in chemical mass along a path of length L

The characteristic travel distance for a chemical in the environment can be calculate using the chemical's estimated residence time in the atmosphere along with speed and direction of the moving phase. The characteristic travel distance in the atmosphere can be calculated finding the distance at which the concentration has reached 36 percent of the initial concentration (Bennett et al. 1998). This can be calculated as:

$$\text{characteristic length} = 0.23 * \text{wind velocity/loss rate}$$

where:

characteristic length	=	distance at which 63 percent of the mass in the air cell has been removed
wind velocity	=	average wind velocity (m/d)
loss rate	=	loss rate from the atmosphere from transformation and depositional processes (1/d)

The 0.23 term approximates the effects of dispersion but dispersion and diffusion are not explicitly modeled in the above calculation. Gifford and Hanna (1973) have shown that the yearly average concentration in a simple box model is proportional to the source strength in mass per unit area divided by the wind speed. McKone (1993a,1993b,1993c) has used the Gifford and Hanna work with Benarie (1980) to derive the proportionality constant in this relationship. Multiplying the unidirectional wind velocity by 0.23 accounts for is the changing direction of the wind; in other words, if you averaged the wind in one direction it would be about 23 percent of the wind speed at any time. This factor may underestimate the characteristic travel distance in locations with persistent wind flow in one direction, and as a result, may result in finer grid spacing.

For transformation losses, the loss rate is equal to the reaction rate in the atmosphere which, for first order reactions, is given by 0.693 divided by the half life in the atmosphere. For deposition losses, the loss rate is equal to the deposition velocity divided by the mixing height.

$$\text{loss rate} = (0.693/\text{half life} + \text{deposition velocity/mixing height})$$

where:

half life	=	reaction half life of the chemical in the atmosphere (d)
deposition velocity	=	total deposition velocity including wet and dry deposition to soil, water, and vegetation (m/d)
mixing height	=	mixing height of the atmosphere (*i.e.,* the height over which pollutants can be assumed evenly mixed) (m)

The atmospheric mixing height is a function of climatic conditions and can be calculated from meteorological data. When determining the characteristic travel distance for a chemical, one may want to make a calculation for each season since the average weather (mixing height, precipitation, mean winds, etc.) may vary significantly. The reaction rates and deposition velocities are chemical specific.

Air dispersion models can also be used to locate system boundaries. By plotting x-y spatial coordinates along with air concentration (z), a map or map-overlay can be generated and used in the same way that a topographical map is used for identifying natural boundaries. The key to using dispersion models or characteristic travel distance for estimating boundaries is deciding what change in concentration can be considered significant. Even if the model gave perfect information, variation in field measurements and imprecision in analytical equipment would likely require a 10 percent to 50 percent change in concentration before the concentration difference between two places on a map could be considered statistically significant (Eiceman et al. 1993). This coefficient of variation increases as the environmental concentration approaches the experimental detection limit of the equipment.

However, it can be safely assumed that multimedia models do not give perfect information. An international group of expert model developers and model users recently concluded that a reasonable estimate (admittedly subjective) of model accuracy for multimedia pollutants was a factor of three. This factor is expected to increased by an additional factor of two each time the pollutant crossed a compartmental interface (Cowen et al. 1995). Thus, as the pollutant moves away from the source through adjacent compartments in TRIM.FaTE, the distance across each compartment should be increased (*i.e.*, reduce resolution with increased distance from source). This characteristic is intuitive in that at some distance from the source, the pollutant will become a regional or global pollutant and one will no longer be able to directly link the pollutant back to the original source.

C.2.3 POPULATION BOUNDARIES

Population mobility boundaries take into account additional information about the habitat of the target and the different locations in which the target is likely to be during an exposure event. Population mobility boundaries are comparable to natural boundaries except that no physical boundary would be visible on a map. Population boundaries can be used to justify increased complexity of a landscape parcel within a natural boundary or within the range of a bounded target (as described in previous sections). For example, an antelope may spend most of its life foraging in the high desert sage around a munitions storage facility. No natural boundaries exist and physicochemical boundaries may provide more resolution than is

appropriate. If the seasonal foraging area of the antelope can be identified, this information can be used to construct parcels that encompass the animal's range for each season. If that range is large, physicochemical boundaries can be used to increase resolution (more parcels) within the boundaries as necessary.

C.3 REVISITING THE INITIAL MODEL SETUP

This section addresses methods for identifying necessary changes in grid spacing and changes to the external system boundary after an initial TRIM.FaTE simulation and a basic uncertainty analysis have been completed. It is important to determine if any changes to the grid spacing are necessary once an initial run has been completed, keeping in mind the analysis objective, the type of target, and the variance in model results.

If the uncertainty of the concentrations within a compartment is greater than the difference in concentration between adjacent compartments, using a finer grid scale will not increase the information that can be obtained from the model. On the other hand, if the uncertainty is less than the difference in concentration between compartments providing a situation where there is a statistically significant difference in concentration between adjacent compartments of similar composition, then a finer grid size may be appropriate. When considering combining adjacent parcels it is important to also examine environmental characteristics of each parcel. An obvious example where adjacent parcels would not want to be combined is adjacent air parcels over land and water. If the water body is large, then the atmospheric mixing height would be different and as a result, the parcels should not be combined.

For instance, a user might find that the initial simulation did not include a large enough region, and the simulations result in a significant portion of chemical mass leaving one of the system boundaries. In this case, the user might want to consider increasing the scale, if warranted by the model objectives, and completing a new simulation. The user would need to consider whether or not there is a potential exposed population downwind from the site. If there is a sensitive ecosystem, farmland, or marine-harvesting region just outside the suggested model range, the user might want to extend the range to include this area as the chemical may bioaccumulate in the food chain, causing a significant exposure. Also, the user would want to evaluate whether or not the mass leaving the system will result in concentrations above the background level. If not, the user might not want to expand the region. If the region was expanded and no gain in useful information was realized, those parcels could always be removed for future simulations.

C.4 SETTING UP THE MODELING REGION

This section builds upon the principles important to selecting the scenario scale, as presented in Sections C.1 through C.3, and addresses the details of defining parcels, volume elements, and compartments.

C.4.1 DETERMINING PARCELS

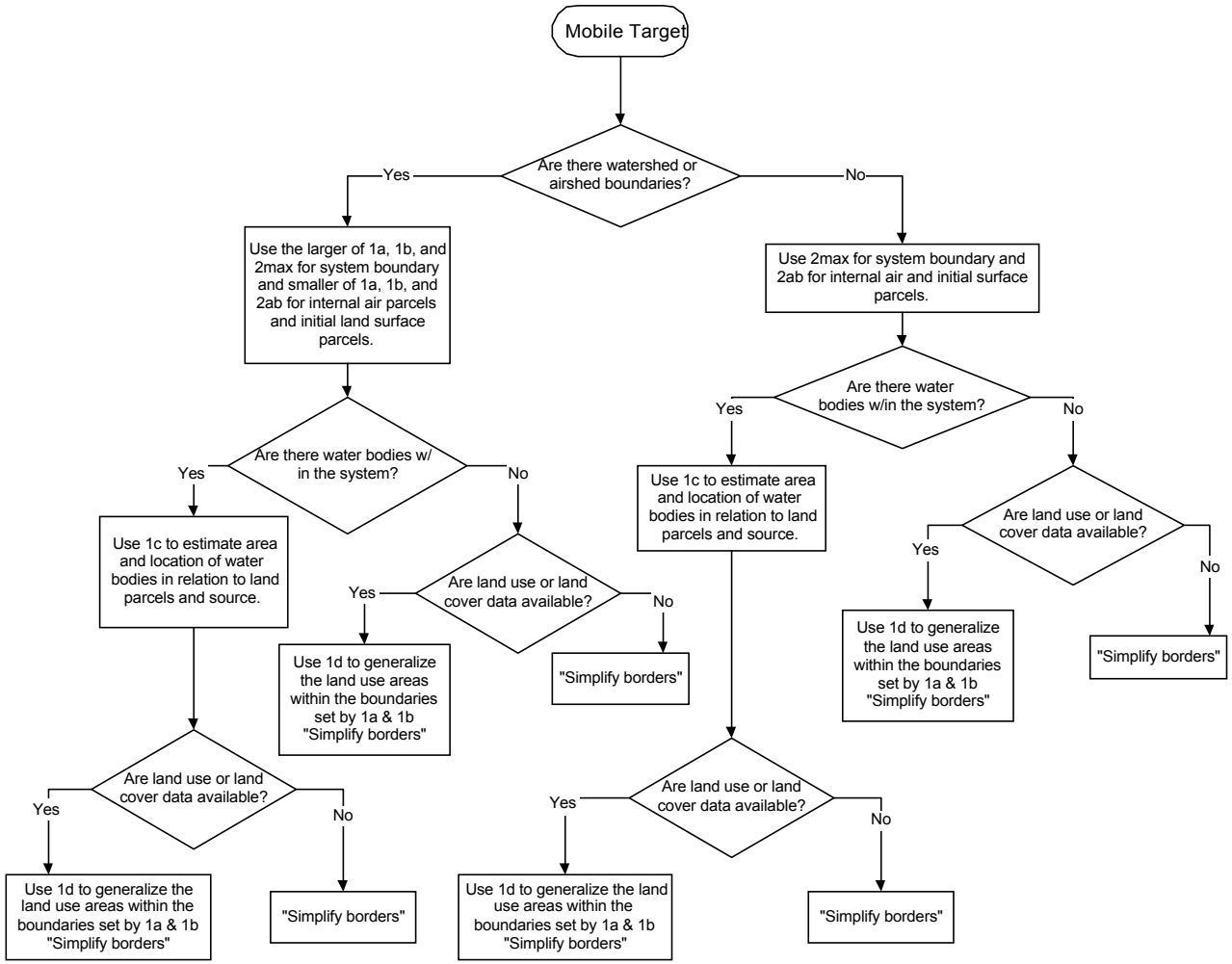
To guide the development of parcels for a given model scenario, a series of decision trees are presented, each for a different model objective. By following the decision tree, appropriate parcels can be determined. After the analysis objective is defined, the dominant target class and chemical(s) of concern can be identified. The target class is then used to select the appropriate decision tree to aid in defining parcels. Refer to Figure C-1 for a mobile target, Figure C-2 for a bounded target, and Figure C-3 for a stationary target. By following the decision tree down a yes/no path, the important boundary types are identified in the order of significance until an adequate level of complexity is attained. The boundary types are listed and coded in Table C-2.

The general pattern within the decision trees consists of a starting point indicated by an oval containing the target class at the top of the page. Following the decision tree, one will come to a diamond that contains a simple question that is answered either yes or no. This may lead to another question or to an action indicated by a rectangle. The action boxes direct the user to one or more of the coded boundary types listed in Table C-2. For mobile targets, the air parcels are defined first. For the bounded and stationary targets, the land surface parcels are defined first followed by the air parcels. When all parcels are defined (no more questions remain on the tree) the process moves to the simplification stage. This stage includes final smoothing of boundary lines, combining adjacent parcels with similar composition, and adding additional parcels around the perimeter of the system.

After the preliminary map of the parcels has been completed based on the decision tree, some slight modifications may need to be made to the map of parcels. Conceptual filtering (also known as best judgment) can be used to transform the curved lines into simple connected polygons while conserving the area and approximate location relative to the source and adjacent parcels. The horizontal area of an air or water basin can be can be estimated using a planimeter by tracing the boundary several times and calculating the average area. The area can then be used to estimate the parcel size. Alternatively, one can simply use a clear ruler and best judgment to straighten the lines. Boundaries based on airsheds can be simplified in the same manner.

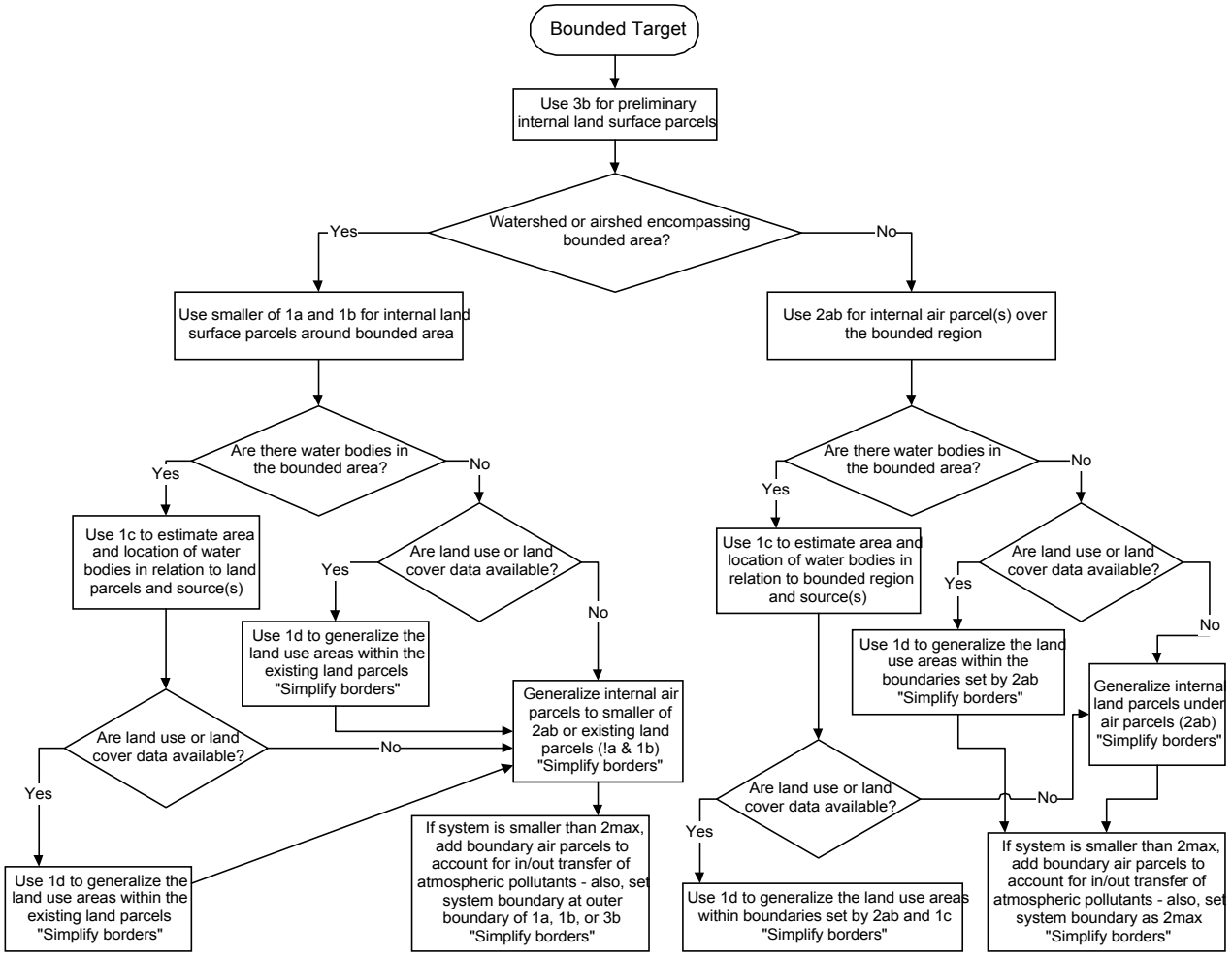
Although the major land types (*e.g.*, forests, urban areas) generally should be considered separately, the actual boundaries of the landscape types may need to be modified to fit the grid structure. In order to capture differences in landscape regions, the land under an air parcel can be split into multiple parcels. This can be an advantage for including rivers and lakes that are narrow or small relative to the air parcel size (differences in atmospheric mixing height over land and water can be ignored if the water body is small). Also, one could include various land uses in a single land parcel if transport differences across various land uses are not significant (*e.g.*, a land parcel may include 90 percent conifer forest and 10 percent deciduous forest). In this case, a hybrid parcel containing a fraction of each cover would be created.

Figure C-1
Mobile Target - Binary Decision Tree for Setting Up Model Region[a]



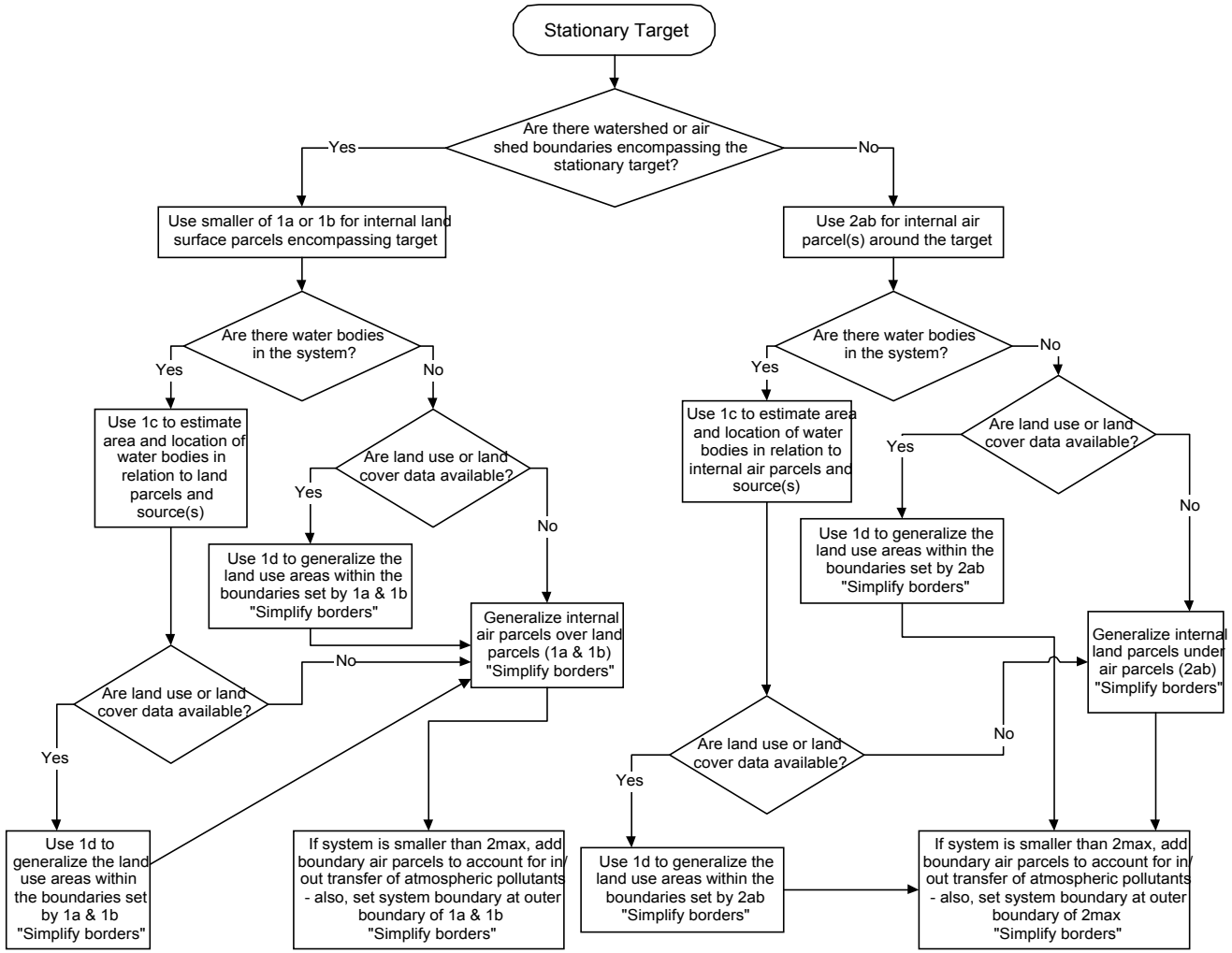
[a] Codes refer to the boundary types referenced in Table C-2.

Figure C-2
Bounded Target - Binary Decision Tree for Setting Up Model Region[a]



[a] Codes refer to the boundary types referenced in Table C-2.

Figure C-3
Stationary Target - Binary Decision Tree for Setting Up Model Region[a]



[a] Codes refer to the boundary types referenced in Table C-2.

C.4.2 DETERMINING VOLUME ELEMENTS

After the parcels have been determined, the volume elements are specified. This step involves determining the appropriate number of volume elements and specifying the appropriate depth for each one. Whereas parcels only represent the modeling region in two dimensions, volume elements add the component of depth, thus representing the modeling region in three dimensions. The development of volume elements represents the final step in specifying the spatial resolution of the modeling region.

If the parcel represents a surface water area, surface water and sediment volume elements may need to be defined. The appropriate depth of the surface water volume element can be determined, for example, based on the average depth of the surface water within that region. An upper and lower water volume element may be appropriate if, for example, the water body is very deep or if different types of fish and other aquatic animals live at different depths. The level of refinement (*i.e.,* number of volume elements used to represent) for a surface water body also depends on the level of detail necessary to answer the modeling questions.

If the parcel represents a land area, the number, depth, and type of soil volume elements will need to be determined. For instance, if the region is in the forest, the soil is unlikely to be tilled and thus the number and depth of soil volume elements would be determined based on the depth the chemical is likely to penetrate. The number of modeled soil layers depends on the desired level of detail and objective of the scenario, but typically three soil layers (represented as volume elements) are considered. For a given land parcel, there is generally a thin volume element composed predominantly of surface soil, reflecting the depth of soil likely to be incidentally ingested by wildlife. The root zone soil layer, represented by a separate volume element, would typically be immediately below the surface soil layer and would reflect the depth to which plant roots are likely to be in contact with the modeled chemical(s). The vadose zone would then extend from the bottom of the root zone soil layer to the ground water surface. If the chemical is likely to penetrate deeply into the soil, a volume element composed predominantly of ground water may also be included.

If the parcel represents air, the number and depth of air volume elements needs to be determined. The boundaries of air parcels do not necessarily have to coincide with the boundaries of the surface water and soil parcels, although to limit the computer resources required for a simulation, the parcel boundaries may be made identical. The number of vertical layers (represented as volume elements) modeled for each air parcel is determined based on the desired level of detail and the modeling objective. For example, if the modeled source has a high release height and only one volume element is modeled, the results are likely to overestimate the deposition of the chemical close to the source. In this case, it would be advantageous to model multiple volume elements representing multiple vertical layers. In contrast, it may be appropriate to model a source with a low release height with one vertical layer.

C.4.3 DETERMINING COMPARTMENTS

Abiotic

Abiotic compartments are determined by the predominant abiotic medium in the volume element within which they are contained. At least one abiotic compartment must be contained within each volume element and, although not typically utilized, the model framework does support multiple abiotic compartments within a volume element. In most cases, the determination of abiotic compartments is an implied step because they are simply defined by the predominant abiotic media within the volume element. For example, if a given volume element is composed predominantly of surface soil, a surface soil compartment would be included in the volume element.

Biotic

The transport of chemicals to biota consists of diffusive and advective processes, through the latter term is rarely used by biologists. Chemicals diffuse into plant leaves from air; chemicals deposit onto plant leaves with particles in air, an advective process. The uptake of chemicals from soil or soil water by plant roots or earthworms is treated as diffusion, though water carries the chemical into the plant (advection). Similarly, chemicals are assumed to enter algae, macrophytes and benthic invertebrates by diffusion. The major advective process is food intake by fish, birds and mammals.

The only transport process within biota that is included in TRIM.FaTE is transport through the plant stem in xylem and phloem fluids. The distribution of chemicals among organs in individual wildlife is not a feature of TRIM.FaTE.

C.5 REFERENCES

Benarie, M.M. 1980. Urban Air Pollution Modeling. Cambridge, MA: MIT Press.

Bennett, D.H., T.E. McKone, M. Matthies, and W.E. Kastenberg. 1998. General formulation of characteristic travel distance for semivolatile chemicals in a multimedia environment. Environmental Science and Technology. 32:4023-4030.

Cowen, E.C., D. Mackay, T.C.J. Feihtel, D. van de Meent, A. DiGuardo, J. Davies and N. Mackay. 1995. The multi-media fate model: A vital tool for predicting the fate of chemicals. Pensacola, FL: SETAC Press.

Eiceman, G.A., N.S. Urquhart, and G.A. O'Connor. 1993. Logistic and economic principles in gas chromatography-mass spectrometry use for plant uptake investigations. Journal of Environmental Quality. 22:167-173.

Gifford, F.A. and S.R. Hanna. 1973. Modeling Urban Air Pollution. Atmospheric Environment. 7:131-136.

McKone, T. E. 1993a. CalTOX, A multimedia total-exposure model for hazardous-wastes sites Part I: Executive summary. Laboratory.UCRL-CR-111456PtI. Livermore, CA: Lawrence Livermore National.

McKone, T. E. 1993b. CalTOX, A multimedia total-exposure model for hazardous-wastes sites Part II: The dynamic multimedia transport and transformation model. UCRL-CR-111456PtII. Livermore, CA: Lawrence Livermore National Laboratory.

McKone, T. E. 1993c. CalTOX, A multimedia total-exposure model for hazardous-wastes sites Part III: The multiple-pathway exposure model. UCRL-CR-111456PtIII. Livermore, CA: Lawrence Livermore National Laboratory.

[This page intentionally left blank.]